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Computer-Aided Approach for Design of Tailor-Made Blended Products

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The majority of chemicals based products are mixtures of two or more substances. It is because a single chemical does not always satisfy the product needs. Mixing or blending is a simple process in chemical engineering, but using suitable chemical substances at right composition in a mixture is important in order to obtain the desired products. Blending process with the appropriate selection of the chemicals could offer advantages, such as, reducing the amount of fossil-fuel consumption and pollutants release to the atmosphere. Product safety and product attributes also could be enhanced by blending. However, the product performance may decline when other chemicals are added. In order to maintain/improve the blended product performance, it is necessary to identify the best product blend with the most appropriate chemicals. Finding the most appropriate chemicals is one of the challenges in chemical blending. The computer-aided approach is a fast and reliable methodology for identifying and selecting the chemicals. Therefore, a systematic computer-aided methodology for chemical blended product design is developed, to identify the most suitable chemicals for blending and formulate blended products that satisfy specific product needs.

In this paper, the systematic computer-aided methodology for product design is divided into four tasks. The first task is to define the design problem, where the product needs are identified, translated into target properties and given target values. In the second task, the required target property models are retrieved from a property model library developed specifically for this methodology. Then, a mixture/blend design algorithm is applied to obtain the mixtures/blends that match the set of constraints (design targets). This algorithm employs a decomposition based solution strategy to solve the mixture/blend problem. The result is a set of blends that match the constraints, the compositions, values of the target properties and information about their miscibility. Finally, the mixture target property values are verified either with experimental data (if available) or by means of rigorous models for the properties and mixtures that require it. The application of this systematic methodology is highlighted through case studies related to the design of blended gasoline and refrigerants, where the objective is to identify blended products that satisfy all the product attributes with at least similar or better performance compared to conventional products.

Keywords: computer-aided approach; chemical blends; product design; gasoline; refrigerant

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